Solution Methods for Large-Scale Nonlinear Problems

Agenda

July 26–28, 2000
Pleasanton, California

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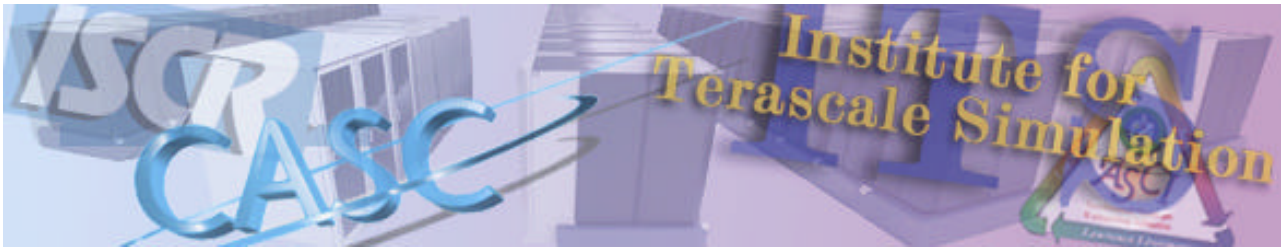

Lawrence Livermore National Laboratory
Livermore, California

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Wednesday July 26, 2000

All proceedings held in the Livermore Room, Four Points Hotel

7:30 – 8:15	**Continental Breakfast**	
8:15 – 8:30	**Welcoming remarks**	David Keyes
	Announcements	Carol Woodward
Topic	**Newton-Krylov Methods**	
Session Chair	**Jim Jones**	
8:30 – 9:00	Xiao-Chuan Cai, *Nonlinearly Preconditioned Inexact Newton Algorithms and Applications*	
9:00 – 9:30	Eric de Sturler, *Analysis of Newton and Newton–Krylov Methods for Nonlinear Problems with Ill-Conditioned Jacobians*	
9:30 – 10:00	Beth Bennett, *Application of Local Rectangular Refinement and Newton–Krylov Methods to Axisymmetric Laminar Flames*	
10:00 – 10:30	**Break**	
Topic	**Newton-Krylov Methods**	
Session Chair	**Carol Woodward**	
10:30 – 11:00	Lea Jenkins, *Newton–Krylov–Schwarz Methods for Hydrology Problems*	
11:00 – 11:30	Jim E. Jones, *Preconditioners for Newton–Krylov Solvers of Richards' Equation*	
11:30 – 12:00	Gerhard Starke, *A Levenberg–Marquard Method for Nonlinear Least Squares Finite Element Computations*	
12:00 –1:30	**Lunch,** FAZ Restaurant Patio	
Topic	**Nonlinear Methods**	
Session Chair	**Van Henson**	
1:30 – 2:00	Dimitri Mavriplis, *Unstructured Mesh Multigrid Solvers for Radiation Diffusion Problems*	
2:00 – 2:30	Craig Douglas, *Getting Burned by Interpolation*	
2:30 – 3:00	Lois C. McInnes, *Matrix-Free Newton–Krylov Methods Using a Hybrid Automatic Differentiation–Finite Difference Strategy*	
3:00 – 3:30	**Break**	

3:30 – 5:00 **Moderated Discussion,** Van Henson and Jim Jones

Can FAS Hold Sir Isaac's Apple?

For some years, the multigrid Full Approximation Scheme (FAS) has been used to solve nonlinear problems in certain applications. It is natural to wonder how FAS compares with Newton's method. Do they both have the same basin of attraction around a solution? How do convergence speeds compare in terms of the convergence factor, the flop count, or the time to solution? Does FAS–FMV insure that the method converges by eliminating initial guesses? Are the methods equally applicable on all problems? Where do Newton–Krylov, Newton–Multigrid and Newton–Krylov–Multigrid fit into the picture?

5:30-7:30 **Reception,** FAZ Restaurant Patio

Steve Ashby, *Introduction to the LLNL Center for Applied Scientific Computing*

Thursday July 27, 2000

All proceedings held in the Livermore Room, Four Points Hotel

7:30 – 8:30	**Continental Breakfast**
Topic	**Applications**
Session Chair	**Jim Jones**
8:30 – 9:00	Ray Tuminaro, *Parallel Unstructured Fully Implicit Finite Element Simulations of Reacting and Non–Reacting Flows*
9:00 – 9:30	Ivan Yotov, *A Nonlinear Newton–Krylov Interface Solver for Multiphase Porous Media Flow*
9:30 – 10:00	Mary Wheeler, *Two-Stage Preconditioners for Fully Implicit Schemes for Multiphase Flow in Porous Media*
10:00 – 10:30	**Break**
Topic	**Problem Formulation**
Session Chair	**Carol Woodward**
10:30 – 11:00	Clint Dawson, *Local Discontinuous Galerkin Methods for Reactive Transport*
11:00 – 11:30	C. Tim Kelley, *An Integro–Partial Differential–Algebraic Equation for Power Consolidation*
11:30 –12:00	Michael Holst, *Some Existence, Uniqueness, and Approximation Results for Nonlinear Elliptic Constraints in the Einstein Equations*
12:00 – 1:30	**Lunch**, Concord Room
Topic	**Applications**
Session Chair	**Peter Brown**
1:30 – 2:00	Carol S. Woodward, *Implicit Solution of Radiation Diffusion Problems*
2:00 – 2:30	William J. Rider, *Development of Newton–Krylov Methods for Radiation Hydrodynamics at Los Alamos*
2:30 – 3:00	Alex Shestakov, *Applications of Pseudo-Transient–Continuation and Newton–Krylov Methods to the Poisson–Boltzmann and Radiation–Diffusion Equations*
3:00 – 3:30	**Break**

3:30 – 5:00 **Moderated Discussion,** Peter Brown and Carol Woodward

To Split or Not To Split: Breaking Up is Hard to Do

Many applications give rise to mathematical models involving multiple equations in multiple unknowns that are nonlinearly dependent on each other. These systems have often been formulated in an operator split or time-lagged manner in order to develop a model numerically solvable within a reasonable amount of time and computer memory. However, with the advent of faster computers, fully implicit formulations are now more tractable. In this session, we will discuss issues related to the decision of when to operator split such nonlinear systems or when to solve them fully implicitly. Are these issues resolved on a problem-by-problem basis or are there some generalities we may find? Is there a dynamic way to tell when operator splitting will be best so that a code may adapt as a solution algorithm proceeds? What experiences have session participants had in developing solution methods for fully implicit and operator split formulations of the same problem?

Friday July 28, 2000

All proceedings held in the Livermore Room, Four Points Hotel

7:30 – 8:30	**Continental Breakfast**
Topic	**Algorithmic Issues**
Session Chair	**Van Henson**
8:30 – 9:00	David Young, *Nonlinear Elimination Applied to Aerodynamic Analysis and Design Optimization*
9:00 – 9:30	David E. Keyes, *Performance Stresspoints for Parallel Implicit Nonlinear Solvers*
9:30 – 10:00	Michael Pernice, *Infrastructure and Algorithms for Nonlinear Problems and Implicit Time Integration on SAMR Grids*
10:00 – 10:30	**Break**
Topic	**Sensitivity Analysis**
Session Chair	**Steven Lee**
10:30 – 11:00	Steven Lee, *Sensitivity Analysis Using Parallel ODE Solvers and Automatic Differentiation in C: SensPVODE and ADIC*
11:00 – 11:30	Linda Petzold, *Sensitivity Analysis and Software for Large–Scale Differential–Algebraic Systems*
11:30 – 12:00	Luc Machiels, *Output Bounds for Partial Differential Equations*
12:00 – 1:30	**Lunch,** FAZ Restaurant Patio
Topic	**Optimization**
Session Chair	**Peter Brown**
1:30 – 2:00	Omar Ghattas, *PDE Solvers and PDE Optimizers: Similarities and Differences*
2:00 – 2:30	George Biros, *All–At–Once Techniques for Optimization of Systems Governed by Time–Independent Partial Differential Equations*
2:30 – 3:00	Stephen Vavasis, *Combining Nonlinear CG with Truncated-Newton CG*

3:00 – 4:00 **Moderated Discussion,** David Keyes and Steven Lee

Sensitivity: Politically Correct or Scientifically Necessary?

There are several trends in scientific computing that are focusing our attention on the use of sensitivity analysis and optimization for simulations: advances in mathematical formulations and algorithms that make it practical to solve large-scale problems, interest in reducing the complexity of computational models, new methods and tools for computing sensitivity information, and an increasing dependence on simulations for policy support or design decisions. In this session we wish to pool attendee wisdom on practice and propaganda concerning sensitivity analysis and optimization. For example, how are the verification and validation mandates of various programs being met today by sensitivity analysis, or how should they be met? Why is optimization well developed in some areas (e.g., weather modeling, aerodynamic design) and not yet developed or much discussed in other areas? What are the relative advantages of the many distinct techniques for computing derivatives in different problem limits (e.g., small vs. large number of parameters or constraints)? Are there any good "poster children" for sensitivity analysis or optimization and, if so, where are they?